











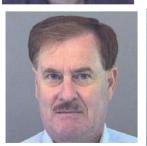




FY01 Dept. Review





















We have a lot to cover.



Introductions

New Staff

Overview

- Scope/Highlights
- Funding

Particulars

- Greg Bessette
- Archie Farnsworth
- Paul Demmie
- Paul Taylor
- Ray Bell
- Dave Crawford
- Stewart Silling
- Marlin Kipp
- Rebecca Brannon

First, meet the new staff.

Greg Bessette



- BS ME University of Florida, MS Eng. Mechanics – University of Florida PhD Eng. Mechanics – UT Austin
- 8 years @ Eglin AFB (concrete penetration, explosive cratering, structural response to blast loading)
- Current work assignment: NMD, Zapotec

Jill Rivera



- BS ME U. of Kansas, MS ME UNM
- 11 years @ SNL (SW development: solid model interrogation for manufacturing, NG tube expert system, stockpile tester design and deployment)
- Current work assignment: W76 Radar Tools, W76 AF&F Cable Tools

Next we have an ...

Introductions

New Staff



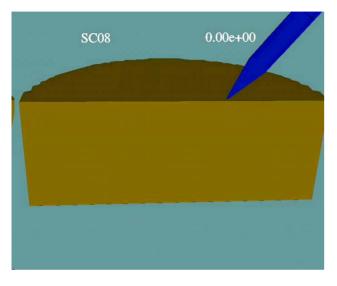
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We historically do...

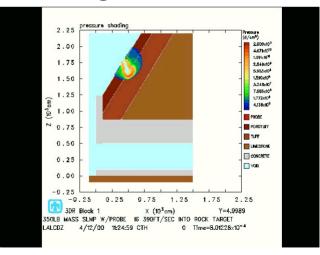


dynamic

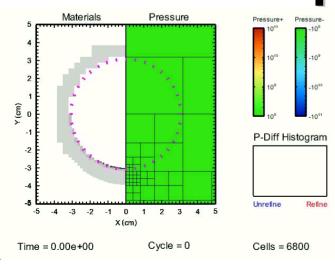
SHOCK PHYSICS

Time=0.

large deformation

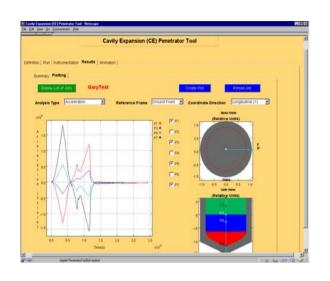


high strain-rate

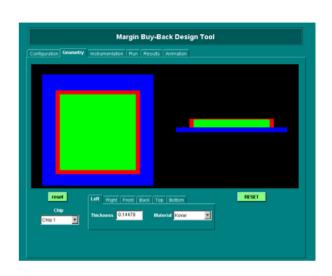


materials

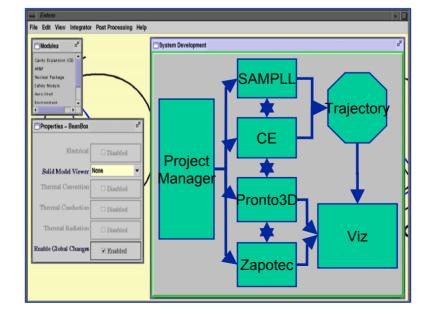
and we do ...



M&S Tools and Frameworks

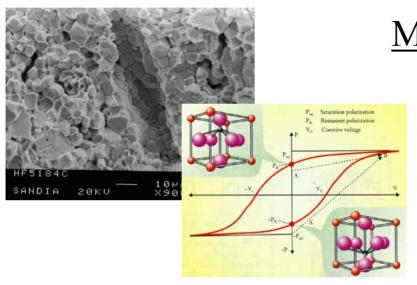








In this context, we research...

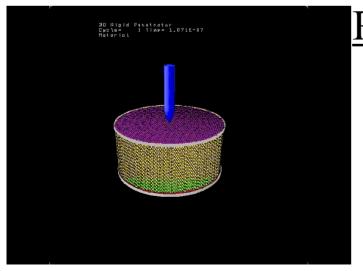


Material Models

- brittle
- porous
- multi-constituents
- multi-phase
- damage
- macrostructure
- microstructure



Rebecca



Peridynamic Theory

- same integral equations apply everywhere
- even in discontinuities, like cracks
- lends itself to mesh free methods

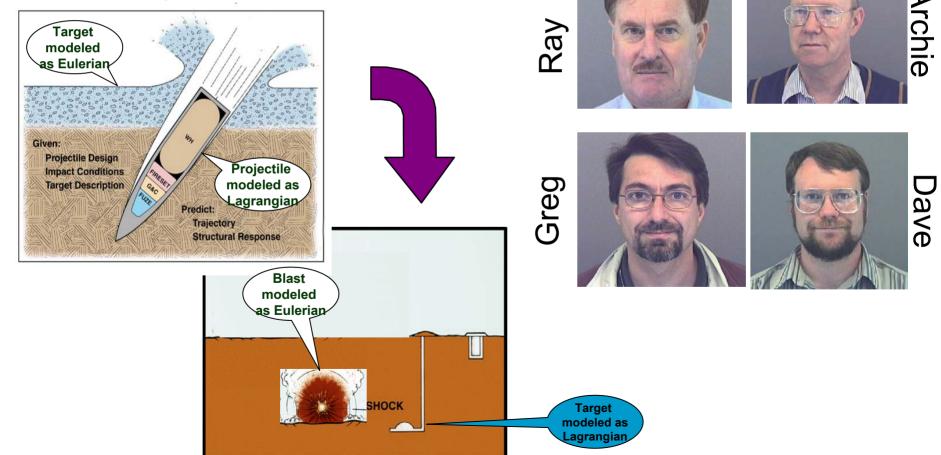


Stewart

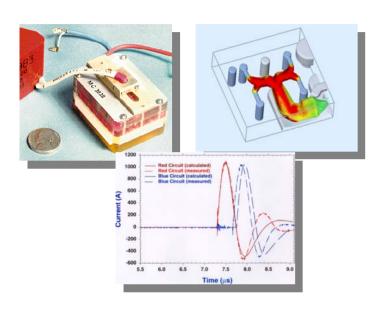
We develop ...

Earth Penetrator Technologies

- "holy grail" of shock physics
- coupled codes (splat/bang & rattle)
- many variants



We apply ...



Firing Set

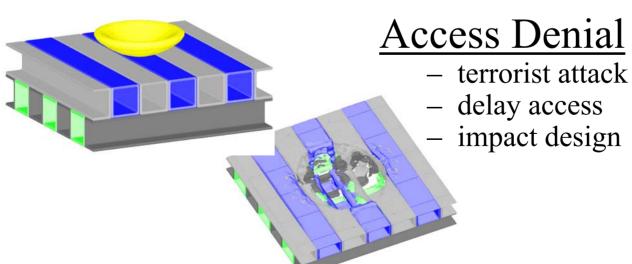
- electromech. model
- model explosives, pzt
- aged materials

delay access

impact design



Paul



Marlin



Jason

We support ...



Paul



Bob

Production CTH

- Interface with user community(> 260 licenses, 1000 users)
- Conduct user training classes
- Code debugging
- Configuration management
- Large and growing number of operating system
- Major releases, code updates
- Documentation
- Telephone support



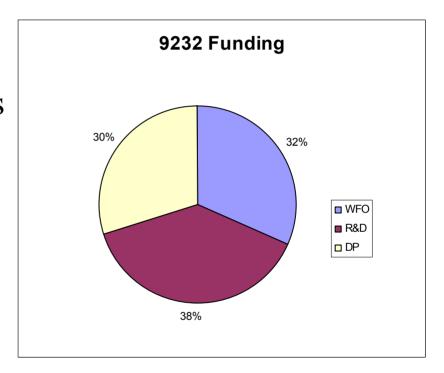
Millie



Marilyn

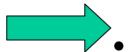
Our funding...

- is based on ~25 related projects
- amounts to >\$3 million, plus additional walk-in work
- is balanced across
 - Research (R&D/DP)
 - Development (R&D/DP/wfo)
 - Application (DP/WFO)
 - Support (DP/WFO)
- supports collaborative work, primarily with 9231
- comes from internal and external sources



And now for the meat!

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Greg Bessette



May 30, 2001





FY01 Projects

ZAPOTEC

Corporate Lethality Program (CLP)

ZAPOTEC: Overview

- Development of a coupled Euler-Lagrange capability
 - Directly couple CTH and PRONTO3D codes

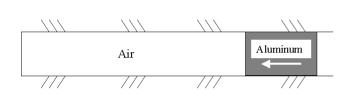
 Coupled approach allows solution of a broader range of problems

ZAPOTEC: On-Going Efforts

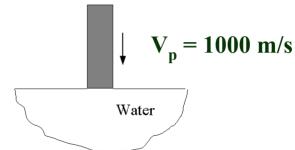
- Software Development
 - Developed more user-friendly command file
 - Consolidation of code for CVS implementation
- Validation and Documentation
 - Pull together suite of example problems
 - Develop accompanying documentation
 - Should provide guidance for performing ZAPOTEC analysis

ZAPOTEC: Example Problems

Gas Piston

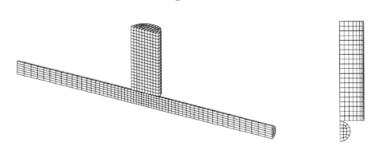


Tungsten Rod Impacting Water



Aluminum Cylinder Impacting Tungsten Rod

$$V_p = 144 \text{ m/s}$$



Tungsten Rod Impacting Moving RHA Target

$$V_p = 2600 \text{ m/s}$$

$$V_t = 330 \text{ m/s}$$

$$\theta = 30 \text{ deg}$$

ZAPOTEC: Future Efforts

- Consider additional example problems
 - Earth Penetrating Weapons
 - Anti-armor Applications
 - Air Blast Loading on Concrete Structures
 - Soil-Structure Interaction
- Software Development
 - Add support for additional PRONTO element types

Corporate Lethality Program: Overview

• Tri-Lab code validation effort for hypervelocity impact applications

• Supports National Missile Defense initiative

- Considers wide range of engagement scenarios
 - Variations in impactor and target configurations
 - Both 2D and 3D code validation

Corporate Lethality Program: On-Going Efforts

- Program is just beginning
- Currently focused on modeling simplified 2D configuration
 - Pre-test calculations completed using CTH

Awaiting results of first test, CLP-1

Witness
Plate

Impact Velocities: 6 and 11 km/s

Ti-6Al-4V Flyer Plate

0.8 mm Thick x 17 mm Diameter

2.5 mm Thick Al Bumper Plate

4 mm Thick Al Witness Plate

Plate Offsets: 75, 100, 150 mm

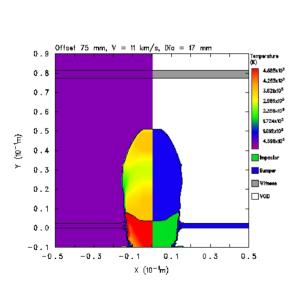
VISAR Records

Corporate Lethality Program: Temperature and Material Plots

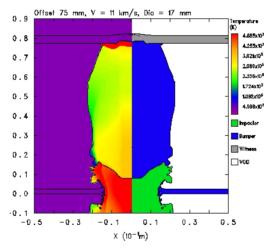
Impact Velocity: 11 km/s

Flyer Diameter: 17 mm

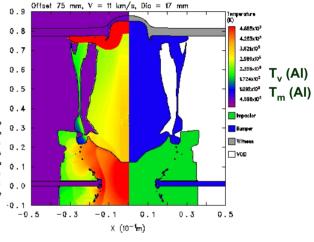
Plate Offset: 75 mm



 $t = 4 \mu s$







$$t = 12 \mu s$$

For Reference:

T_m (AI): 933 K

 T_{v} (AI): 2330 K

T_m (Ti): 2075 K

 T_{v} (Ti): >3075 K

Corporate Lethality Program: **Future Efforts**

- Near term
 - Model experiment CLP-1
 - Requires full 3D calculation

- Long term
 - Perform pre-test calculations for more complicated 3 configurations. e.g







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Archie Farnsworth



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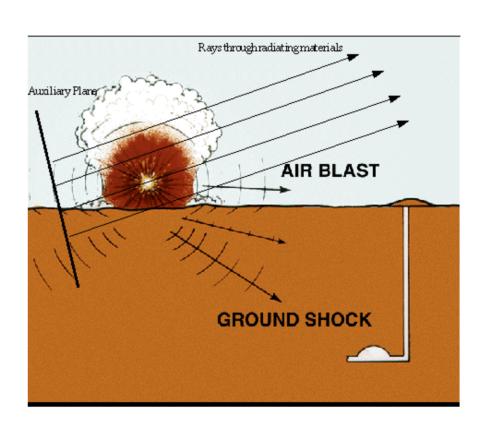


FY01 Projects

- Optical Signal Post Processor for ALEGRA for 5700 and 6500
- Laser Driven Flyer Plates for EOS Studies (especially for thin structures) LDRD
- Navy Kill Vehicle Lethality Study for Specified RV's for 15400 and Navy
- Smaller projects: (1) CTH energy balance routines,
 (2) NUDET in cavern, (3) Lethality of X-ray flux on RV

Detection and Location of Nuclear Detonations: A Sandia Mission

- Current sensors, algorithms: air burst data, old designs
- Target set now includes hard deeply buried targets requiring ground bursts, for which there is no data
- Modern weapon designs produce different signals
- New data is unlikely, so ... computation must suffice!



Physics of Optical Signals from NUDETs

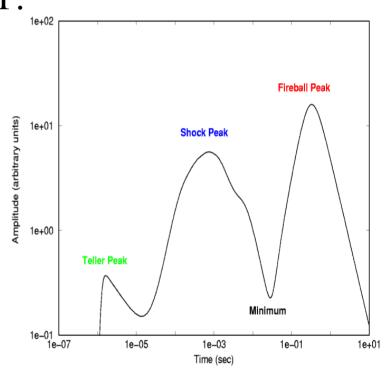
• Three pulse signal from NUDET:

Teller light - air fluorescence (Gamma rays, Neutrons)

Shock light - shock wave in air

Fireball light - prev. heated air

• Trigger on rise of shock peak: most complex, uncertain part



The Optical Signal Post Processor

• Required Input:

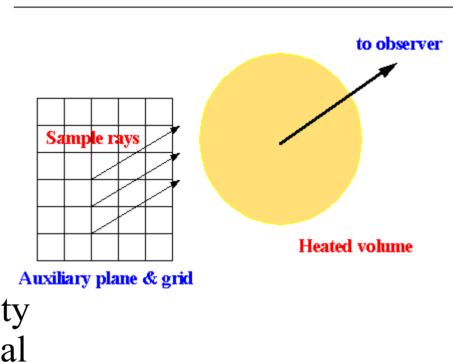
Direction to observer ALEGRA data Air optical opacities

• The Post Processor:

Define sampling rays Sample data along rays

Compute radiative intensity

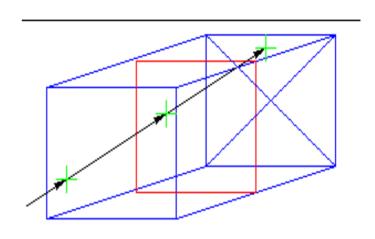
Sum contributions to signal



• Output: Data to compute quantitative sensor response

Computation of Radiative Intensity

 Path through arbitrarily connected cells of ALEGRA grid: Find intersections with face Save distance through cell



 Computation of Ray Intensity on emergence from grid: Solve Eq. Of Rad. Transfer through succeeding cells

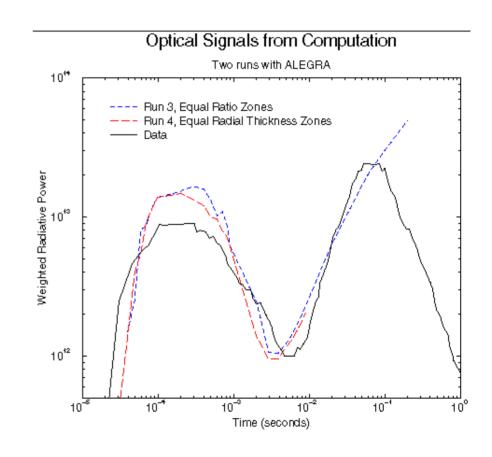
$$\frac{1}{c}\frac{\partial I_{\nu}}{\partial t} + \frac{\partial I_{\nu}}{\partial s} = \rho \kappa_{\nu} (B_{\nu} - I_{\nu}) \quad \text{through cell:} \quad I_{\nu} = I_{\nu}(0)e^{-\tau} + B_{\nu}(1 - e^{-\tau})$$

$$\text{where} \quad \tau_{\nu} = \int \rho \kappa_{\nu} ds = \rho \kappa_{\nu} \Delta s \quad \text{through acell}$$

Post Processor Present Status

- Main features reproduced but lacking detail
- Timing of minimum indicates yield
- Physics Still Needed:

 Preconditioned Air
 Radiative Losses at
 long wavelength



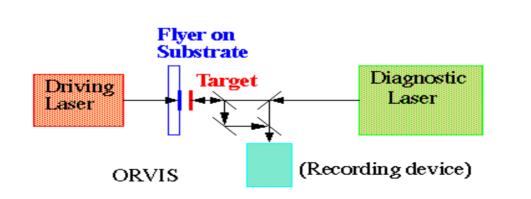
Laser Driven Flyer Plates for EOS Studies

• Needs:

Methods to examine "thin" materials Less costly methods for any material

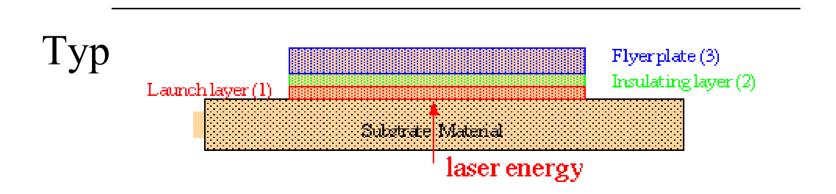
• SNL Assets:

High power lasers to drive flyer Excellent measurement tool (ORVIS) Developed computational tool (CTH)



Computational Capability

- CTH modifications allow laser energy deposition for normally incident rays, following the CTH grid
- Energy Deposition algorithms for laser absorption in the metallic or plasma state

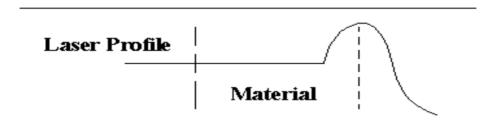


1-D Variations of flyer assembly

- Varying launch layer 1, constant sum of layers (1) + (2) Chose value of .25 microns (0.1 - 5.0 range)
- Fixed launch layer 1, varying layer 2 thickness
- Varying layer 2 thickness, at greatly reduced thermal conductivity
- Results: Very large insulating layer to cool back side All cases show cool front (impact) side

Variations in 2-D

• Laser deposition profile variations:
Flat center, Gaussian roll off at edge
Flat center, high ridge at edge, then roll off



• Result: Large variations in deposition profile produce barely noticeable effect in foil flatness

Suggests little sensitivity to details of profile





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Paul Demmie



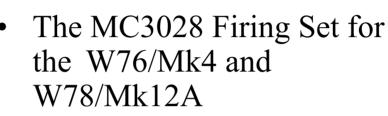
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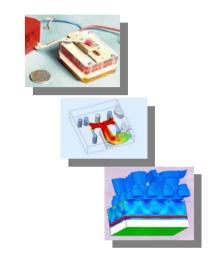


FY01 Projects

- The Entero Earth Penetrator Toolkit
 - Funded by CSRF

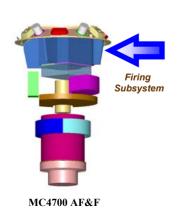


Funded by ESP



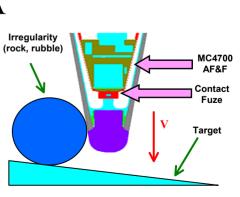


- Funded by DP
- The W76-1/Mk4A:
 Collisions with Obstacles and Impacts with Irregular Targets
 - Funded by ASCI



Entero Earth Penetrator Toolkii

Analysis Codes



Goal of the ENTERO Project

To develop a flexible environment for the design and analysis of complex systems in

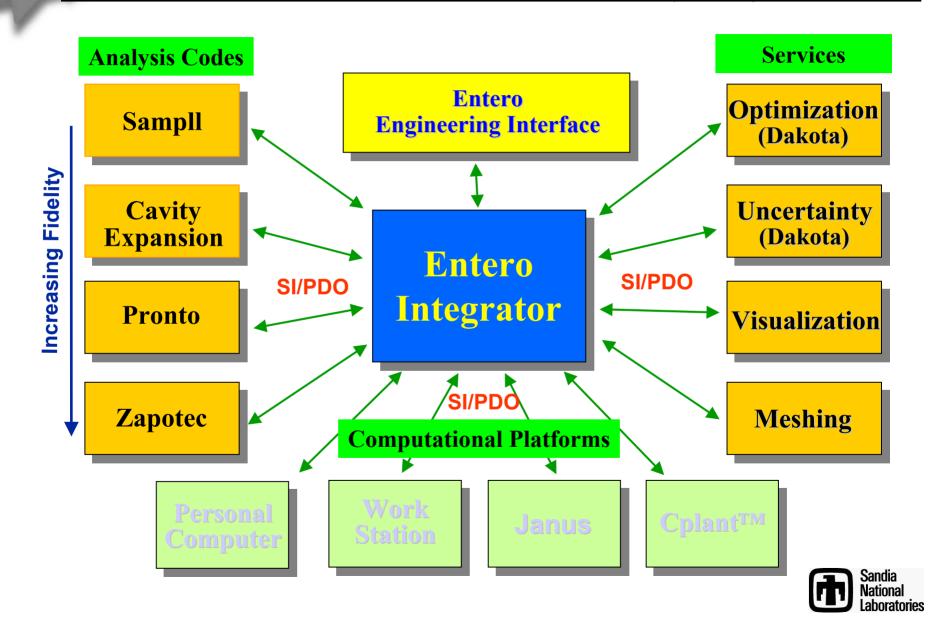


diverse environments from a system-oriented, module-oriented point of view using models with varying degrees of fidelity

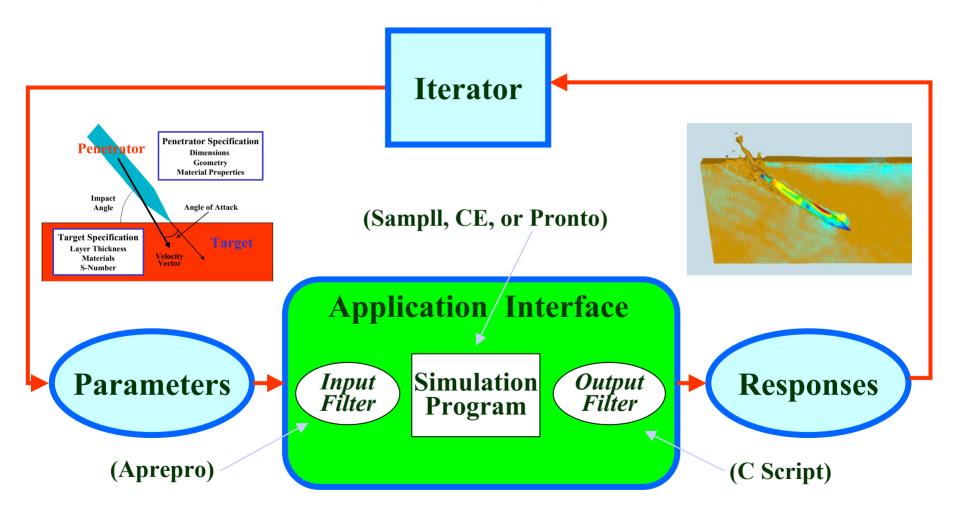


and accessed by means of a web-like user interface.

The Entero Earth Penetrator Toolkit (EPT)



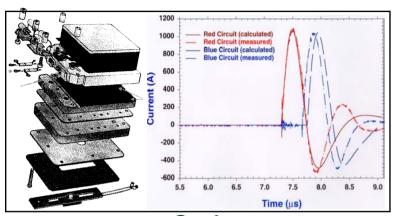
Optimization and Uncertainty in the Entero EPT Using DAKOTA



Accomplishments for the Entero EPT

- Completed a top-level design of the Entero EPT
 - Summarizes vision of the mature toolkit
- Developed a prototype for critique by targeted users
 - Team effort with Joe Castro, Luis Hernandez, Dave Miller
- Developed methodology for integration of penetrator analysis codes with DAKOTA
- Modified Sampll code for integration in the EPT
 - Includes damage criterion used by designers
- Illustrated methodology with example problems
 - Summarized in paper Optimal Design of Complex Systems
 Using the Entero Code System

Modeling the MC3028 Firing Set and Simulating Its Performance



Goal

 Create a comprehensive, coupled 3-D electromechanical (EM), age aware model of the MC3028 slim-loop ferroelectric (SFE) firing set

Approach

- Use EMMA, a 3-D Lagrangian-Eulerian computer code which includes electromagnetic field calculations and attached circuits
- Create computational model
- Simulate performance

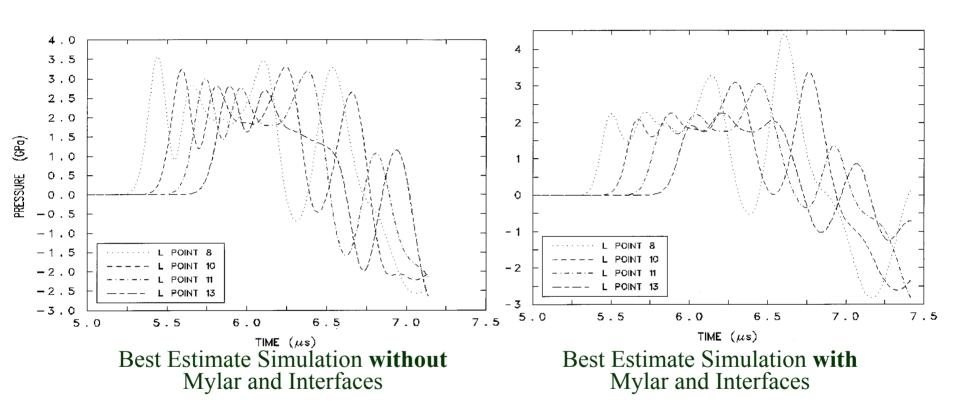
Customer/User

George Clark

Accomplishments

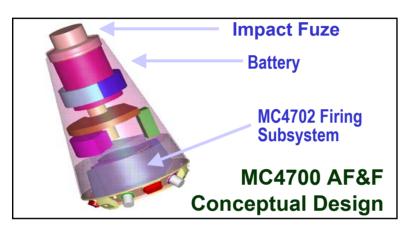
- Met all customer expectations by end of FY00 including documentation
- Obtained new SFE data (Pandora's Box)
 - PBZT conductive at high pressures, fields
- Added mylar layer and interfaces between SFE elements to calculate correct pressures in SFE stack (full-stack and quarter-cell models)
 - Possible because of Cubit development and teaming
- Developed new EM model for SFE material
 - Includes strain and electric field dependence
- Obtained new data for validation process
 - Preliminary comparisons look good

Comparison of Pressures in SFE Stack



These results show effects on pressure of including a 3-mil mylar layer between buffer plate and SFE stack and RTV-foil interfaces.

Analysis for Design of the MC4700 Replacement AF&F for the W76-1/Mk4A



Purpose

- Analyze impact of Mk4 reentry body (RB) into targets to predict impact-fuze performance
- Determine time MC4702 firing subsystem has to initiate detonators before some component critical to nuclear detonation becomes inoperable (timing requirement)

Customer/User

Randy Harrison

- Create CTH model of W76-1/Mk4A
- Simulate impacts using CTH
- Determine timing requirement

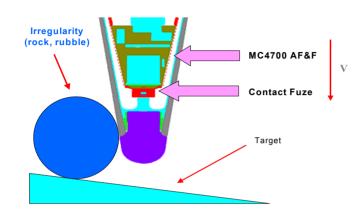
Accomplishments

- Developed analytical method and criteria to assess damage to critical components (MC4702 and nuclear explosive package)
- Completed simulations into hard and soft targets for eight representative velocity-angle (V-γ) points
- Determined that fuze operates at all V-γ points
- Determined timing requirement

FY01 Milestones

- Develop a timing requirement (first quarter)
- Document in presentation (second quarter)
- Document in SAND report (fourth quarter)

Collisions of the W76-1/Mk4A with Obstacles & Impacts with Irregular Targets



Issues

- Simulations to support DSW customers have been performed with RB impacting a perfect target to develop a timing requirement for a firing subsystem
- DSW customer wants to know the effects of collisions with obstacles and impacts into irregular targets

Customer/User

Randy Harrison and Brad Godfrey

Approach

- Create CTH model of W76-1/Mk4A and template input for collisions and impacts
- Simulate collisions and impacts using CTH
- Analyze results and document

Accomplishments

- Summarized past hydrodynamic analyses
- Developed an initial target suite
- Created CTH models for simulations
- Completed base case simulation and one simulation of impact into irregular target

FY01 Milestones

- Develop an initial target set (first quarter)
- Create CTH models (second quarter)
- Complete CTH simulations (third quarter)
- Document results (fourth quarter)

In Summary ...

- I have taken a proactive role in the Entero Project by developing an Earth Penetrator Toolkit emphasizing optimal design with uncertainty and
- I remained agile and responsive to the Defense Program's needs for Stockpile Stewardship on the W76 by
 - modeling and simulating the MC3028 firing set for ESP
 - performing analyses to develop a timing requirement for the firing subsystem in the W76-1 Replacement AF&F and
 - determining effects of obstacles and irregular targets on weapon performance.



FY01 Department 9232 Review

Paul A. Taylor



May 30, 2001





FY01 Projects

- CTH Development Project Leader
 - Contribute to CTH Development
- Constitutive Model Development
 - In support of:
 - Reactive Fragments Program
 - PBX Modeling (ASCI Program)
- Miscellaneous Tasks

CTH Development Project Lead

Mileposts

- Distributed latest version (FEB01) of CTH to external customers with:
 - Adaptive Mesh Refinement (AMR)
 - Spymaster Graphics (must be used for 3D AMR)
 - New EOS, Strength, & Damage Models
 - New/Updated Features
 - Boundary Conditions
 - Convection Options
 - Limited Distribution (NT version) via FTP & Encryption
- User Support & Training
- New User Licenses Issued

FEB01 CTH: EOS Models

- Baer Viscoelastic Model
 - describes time-dependent hydrostatic response according to a Maxwell viscoelastic model
 - examples: PMMA, Kel-F
- Grady P-^{\lambda} Geological Mixture Model
 - describes nonequilibrium compaction of a mixture of geological materials
- Time-Dependent JWL Model
 - modification of conventional JWL EOS to include delayed energy release
 - example: Aluminized Explosives

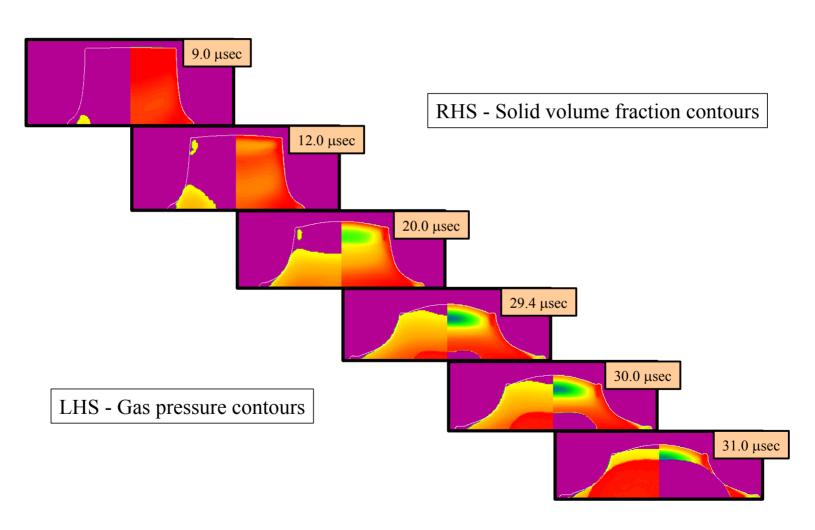
FEB01 CTH: EOS Database Improvements

- New EOS Sesame Tables
 - Plastics:
 - -Teflon, PMMA
 - Carbon
- Improved/Corrected Material Parameters
 - Arrhenius Reactive Burn (ARB) Model:
 - -Teflon, PMMA, Graphite Epoxy, Quartz Phenolic
 - Phase Transition (PTRAN) Model:
 - -Iron (alpha, epsilon), Tin (I, III), & Titanium (alpha, omega)
 - Improved fits of MGRUN & HVRB Materials
- Available to CTH and ALEGRA

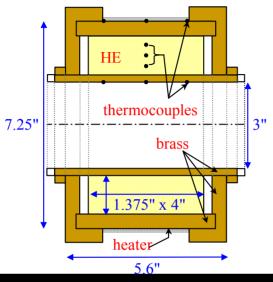
FEB01 CTH: EOS/Strength/Damage Model

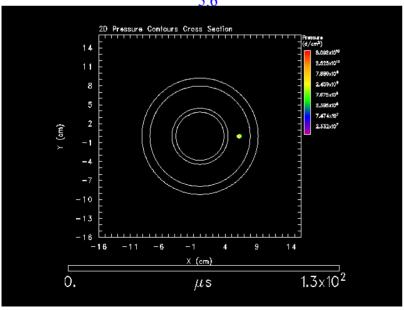
- CDAR (Coupled Damage And Reaction)
 - Consists of 3 interacting modules (VEP, TDD, MP)
- VEP (Viscous-Elastic-Plastic) Deviatoric Response
 - Generalized Maxwell viscoelastic model
 - Strain-rate dependent plasticity
 - Response modified by damage from TDD module
- TDD (Tensile Damage & Distention)
 - Two damage processes: particle decohesion and binder scission
 - Describes viscoelastic-viscoplastic porosity evolution
- MP (Multiphase) Burn
 - Models energy release in porous energetic materials
- CDAR simulates SDT, DDT, and XDT behavior

CDAR Example: 2-D XDT Simulation



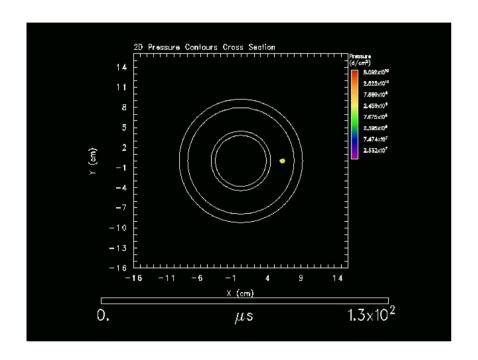
CDAR Example: HE Cook-off

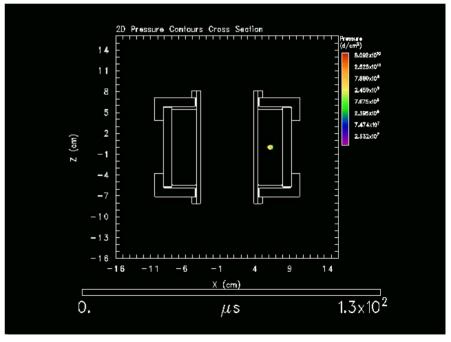




- Simulation of cook-off experiment for PBX-9501 explosive (HE)
- Experimental configuration:
 - 2.5 Kg HE contained in brass cylinder annulus
- Test conditions:
 - Temperature increased to
 150C for 2 hrs, to 180C for
 ~10 hrs
- Result: Violent Reaction

HE Cook-off: THE MOVIES





Distribution of FEB01 CTH

- Limited distribution of CTH for NT
 - Electronic Distribution
 - Runtime Security
- Encryption of CTH Executables, Documentation, and Data
 - Encrypted CTH distributed via FTP using Triple Data Encryption Standard (TDES)
- Runtime Security:
 - Ties execution of CTH to specific computer
 - No hardware lock (dongle) required

User Support & Training

- Alpha version of FEB01 CTH
 - Released to DoD community in September, 2000
 - Bugs identified and fixed
- FEB01 CTH Distributed April, 2001
 - Offered CTH Basic User's Class March, 2001
 - 75% Class Attendees were DoD or DOE
 - Sponsored EOS Class w/J. Kerley March, 2001
- Respond to CTH user queries/problems via telephone & e-mail

Constitutive Model Development

- In support of "Reactive Fragments" Program
 - WFO program with NSWC-DD
- Model constitutive behavior of Al/PTFE subjected to impact and penetration of Al & Steel targets
 - PTFE: Polytetrafluoroethylene (Teflon)
 - Al/PTFE exhibits mechanical loading induced reactivity ~ 20% that of TNT detonation
 - Al/PTFE composition: 25% (wt.) Al in Teflon matrix

Al/PTFE Mechanical Behavior Requirements

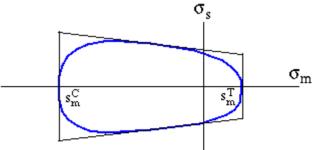
- Pressure Dependent Strength
 - Does pressure dependency exist?
 - Shear-induced dilatation?
 - If so, Triaxial Stress data required
 - Data collected at Sandia, NM; Geomechanics Dept.
- Gas Gun & ICE (Isentropic Compression) Data
 - Hugoniot & Spall
 - Wave Evolution Data
 - for Viscoelastic behavior
- Taylor Anvil Test
 - for validation of strength, fracture, & reaction representations

Modifications to CDAR Modules for Representation of Al/PTFE

- Viscoelastic-Plastic Representation (VEP Module)
 - Define a Yield Surface
 - Pressure dependent
 - Different yield points in tension & compression
 - Separate plastic strain measures for tensile & compressive loading states
 - Shear induced dilatation

$$\sigma_s = \text{mean stress}$$

» = von Mises stress



Modifications to CDAR Modules for Representation of Al/PTFE

- Damage Accumulation (TDD Module)
 - Mechanical Damage associated w/ shearinduced heating
 - Preliminary Damage modeling represented by simple "accumulated plastic strain to failure criterion" $\sum_{n=1}^{\infty} \frac{1}{\varepsilon_n^f}$
 - Example:

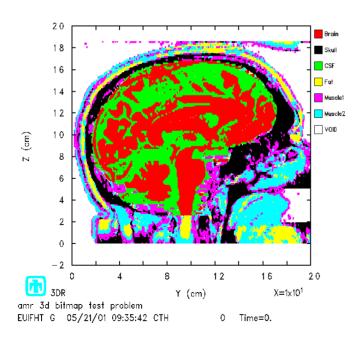
$$\varepsilon_p^f = \varepsilon_p^f(P, \sigma_{vm}, \dot{\varepsilon}, T)$$

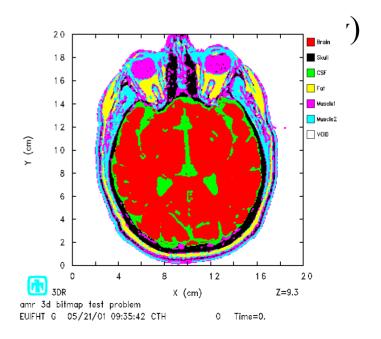
Modifications to CDAR Modules for Representation of Al/PTFE

- Chemical Energy Release (MP Module)
 - Mechanical damage (adiabatic shear heating)
 causes decomposition of Teflon
 - Fluorine released, reacts with Al particles
 - Energy liberated
 - Work in progress in collaboration w/ 9116 staff
 on MP representation of Al/PTFE in CTH

Miscellaneous Tasks

- WFO Program
 - Conduct simulations of impact scenarios
 leading to Traumatic Brain Injury in humans
 - NM Telehealth Proiect (PI: Dale Alverson)





Miscellaneous Tasks

- Manage Consultant Contracts
 - Kerley Publishing: EOS consultation
 - Ben Cole: Consultant for CTH problems on Janus

- Commercial Licensing of CTH
 - Schlumberger Well Services
 - Prime Perforating Systems Limited



FY01 Department 9232 Review

Ray Bell



May 30, 2001





FY01 Projects

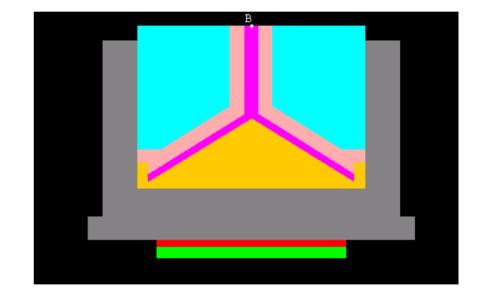
• ISOLATOR Project (MC3347) for George Clark

• ZAPOTEC Coupled Code

CTH

Isolator (MC3347)

- Develop an ALEGRA Model suitable to run EMMA to predict electrical output from the Isolator for SLEP.
- Started with existing Lagrangian model developed by Mark Boslough.
- Added PZT Disc, Lower Steel Disc, Brass Can, Explosive Detonator, and Epoxy Filler.
- Initial runs gave electrical output much lower than expected (pressure at the various surfaces matches experimental results)



Isolator (Cont'd)

- Iterated with Steve Montgomery on PZT parameters.
- Iterated further with Josh Robbins.
- Continuing to work thru ALEGRA issues.
- Latest model uses ALE Blocks for all Lexan parts to prevent mesh tangling at late times.
- Model now has 76 zones across the PZT and 4 zones across the Bond Layer.

ZAPOTEC

- Coupled Code (CTH/PRONTO) written in Fortran 90.
- Original Code not suitable for Massively Parallel Computer Platforms.
- Project with several others to modify the code to work on Massively Parallel Platforms.
- Modifications on set of variables that need to be exchanged between CTH and PRONTO.
- Reduced the number of CTH materials required for Lagrangian Material Insertion.
- Modified CTH to NOT call the EOS for Lagrangian Materials.
- Added Momentum Transfer using Half Index Shifted (HIS) Momentum scheme (PRONTO to CTH).

ZAPOTEC (Cont'd)

- Added Mass weighted Stress Deviator Transfer (PRONTO to CTH).
 Consistent with CTH treatment.
- Added von Mises radial return stress deviator adjustment to ZAPOTEC using the strength values from CTH. This prevents including stress deviator values that cannot be supported by the Eulerian materials.
- Participated in a Coupled Code Conference (Sponsored by DTRA) in La Jolla. I was assigned duty as the Eulerian Module Chair (attended with Steve Attaway and Courtenay Vaughan).
- Helped Courtenay install and explain ZAPOTEC at ARL.
- Presented (with Steve) ZAPOTEC Capabilities to CIA.
- Have version that works with the latest Adaptive Mesh Refinement (AMR-CTH) in Conventional and "Genless" modes. Continuing work to allow full AMR capability.

ZAPOTEC: THE MOVIE



CTH – NSWC (Naval Surface Warfare Center)

- NSWC interested in Reactive Fragments (Long time events, out to several milliseconds).
- CTH Time step (DT) is based on sound speed (C) and material velocity.
- DT for advection dominated flow need not depend on sound speed.
- Modified DT determination by adding a multiplier (0.0 < ALPHA <= 1.0) to C based on local conditions (local pressure gradients).
- The maximum ALPHA found in the mesh is kept and the pressure (and stress deviator) gradients are multiplied by this ALPHA squared in the momentum update.

CTH – NSWC (Cont'd)

- The Transmissive boundary condition (1) in CTH also needed to be modified by multiplying the C terms by this maximum ALPHA.
- The speed up for a moving blob of different density air is about a factor of 5.
- We still do not understand why the C dominated DT results in CTH are so poor (compared to the adjusted DT results).

Preconditioning Methodology

$$\partial u / \partial t = -(1/\rho)\partial P / \partial x$$
$$\Delta u / \Delta t = -(1/\rho)\Delta P / \Delta x$$

Find the change in pressure that will yield a change in velocity equal to the sound speed.

$$\Delta Pc = \rho \Delta u \Delta x / \Delta t$$
$$\Delta Pc = \rho C \Delta x / \Delta t$$

Define alpha as a function of local conditions.

$$\alpha = (arbitrary constant) | \Delta P / \Delta P c |$$

Apply suitable limits on alpha and use alpha as a multiplier on the sound speed in determining the new time step.

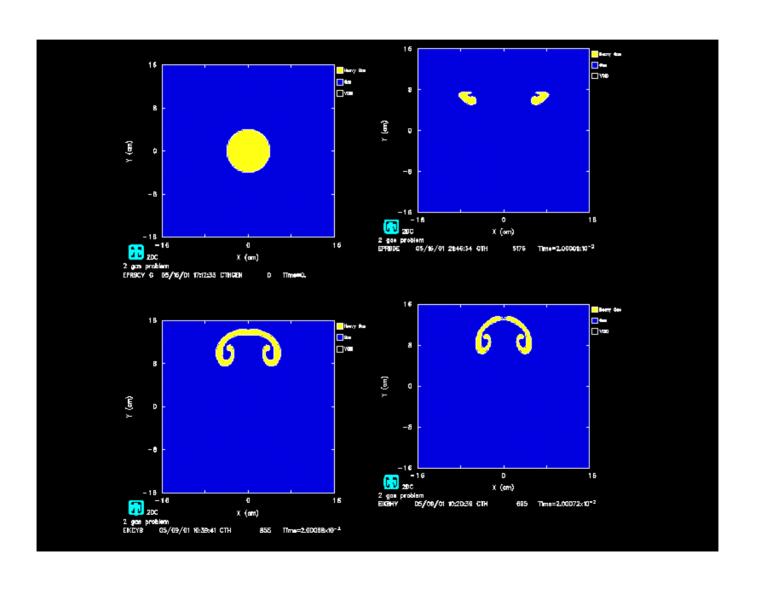
$$\Delta t = \Delta x / (|u| + \alpha C)$$

For consistency the maximum alpha in the mesh must be stored and alpha squared is used as a multiplier in the momentum update.

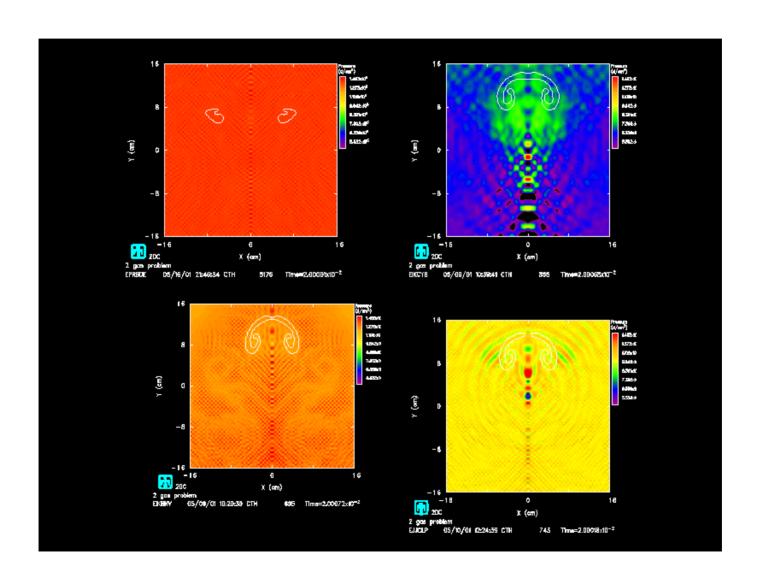
$$\Delta u / \Delta t = -(1/\rho)(\alpha_{\text{max}}^2)\Delta P / \Delta x$$

This same maximum alpha is used as a multiplier to the sound speed in the transmissive boundary condition routine

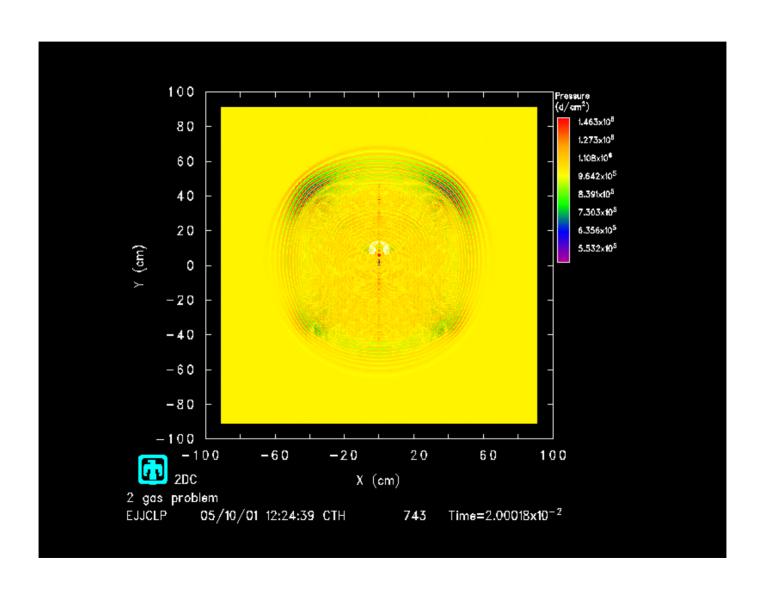
Time Step Control Comparisons



Time Step Control Comparisons



Time Step Control Comparisons



CTH - General

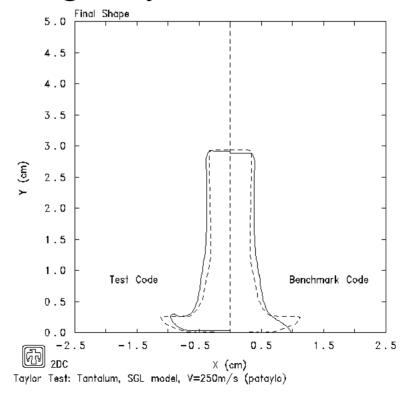
- Tracked down MANY bugs (Tracer Point Errors).
- Assisted other developers with their modifications.
- Created new MMP3 option (essentially a simplified MMP2 that does not require EOS call, MMP3 is now the backup for MMP2 if the EOS call fails).
- Working with AMR-CTH to make it compatible with ZAPOTEC.

FEB01 CTH: Boundary Conditions

Non-stick reflective boundary

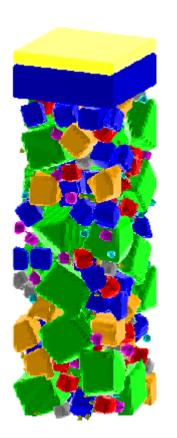
- permits impacting body to "bounce" off rigid

boundary



FEB01 CTH: Boundary Conditions

- Periodic boundary condition
 - Effectively extends material microstructure features beyond mesh boundary
 - Useful for simulating material
 with explicit microstructure



FEB01 CTH: Convection Options

- New Energy/Momentum Convection Options
 - Total Energy Convected (Momentum conserved)

 Option 1: subtract of Metal and with toll-contered velocities

Option 2: Subtract off cell-centered KE
$$KE = \frac{1}{4}m_{i+1/2}[(v_i)^2 + (v_{i+1})^2]$$

- Result: Internal Energy convected w/ KE residual
- Original energy convection option still available
 - Internal energy convected (van Leer), KE ignored, momentum conserved



FY01 Department 9232 Review

David Crawford



May 30, 2001





Overview

- Status of AMR
- Improving AMR usability
 - User's Guide
 - User Training
 - New parallel post-processing capability (spyplt)
- Example 2-D and 3-D AMR CTH calculations
- Performance improvements
- Future and proposed code developments
 - Further enhance improvements
 - Reduce memory requirements

AMR CTH

- Block-based
- Generalization of MPCTH (with multiple blocks per processor)
- Isotropic 2:1 refinement/unrefinement
- Single time-step for all blocks
- User specifies global dimensions of mesh, maximum number of allowed blocks (per processor) and block dimensions (Nx, Ny, Nz)
- Load balance on per-block basis (don't split blocks across processor boundaries)

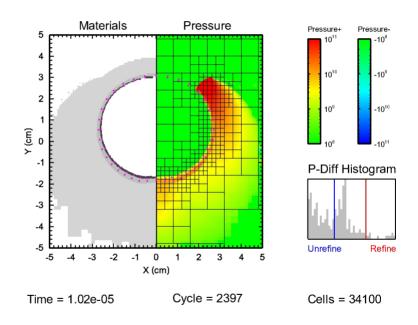
Status of AMR

- AMR version 1.00 has been released externally:
 - includes on-the-fly and post-process visualization using Spymaster.
 - unlimited block allocation (Millie Elrick)
 - user-definable generalized indicators
 - does not include Zoltan or other recent performance enhancements.
- Production AMR will shortly include:
 - significant performance enhancements
 - Zoltan
 - 3-D visualization improvements

AMR Usability generalized indicator syntax

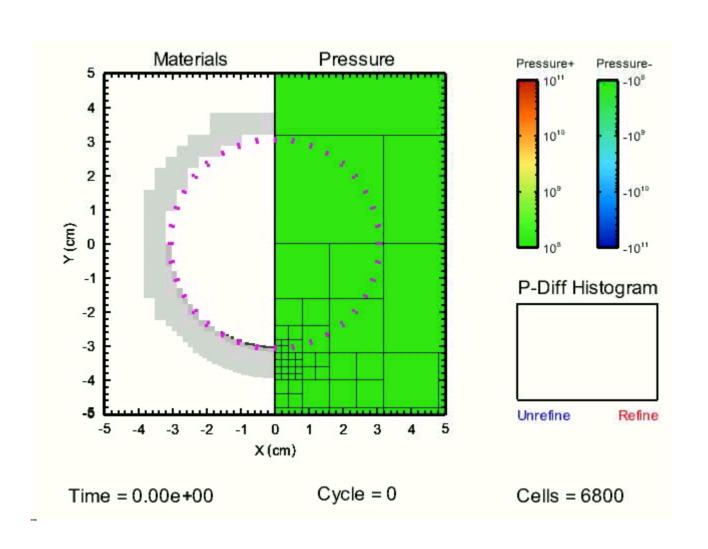
. . .

```
* Use histogram of max.
* pressure difference
* across cell as refine/
* unrefine indicator
indicator
 diff pressure
 vmin 1e8
 logh
 refabove 0.95
 unrbelow 0.5
 ton 0.5e-6
endi
```

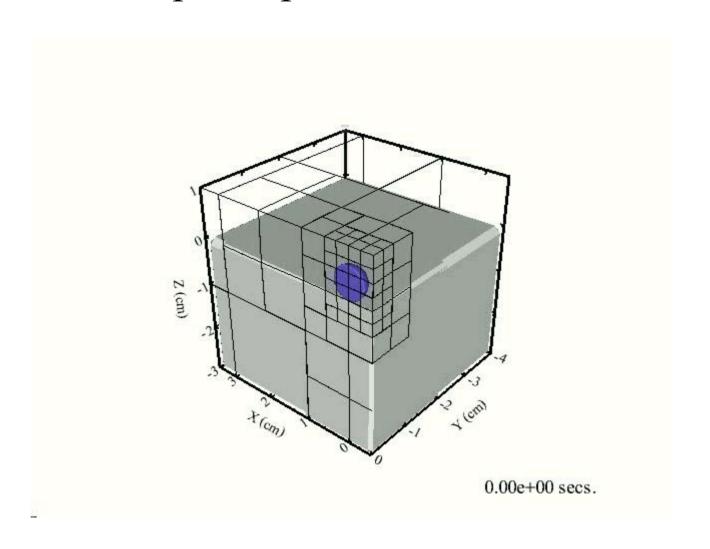


enda

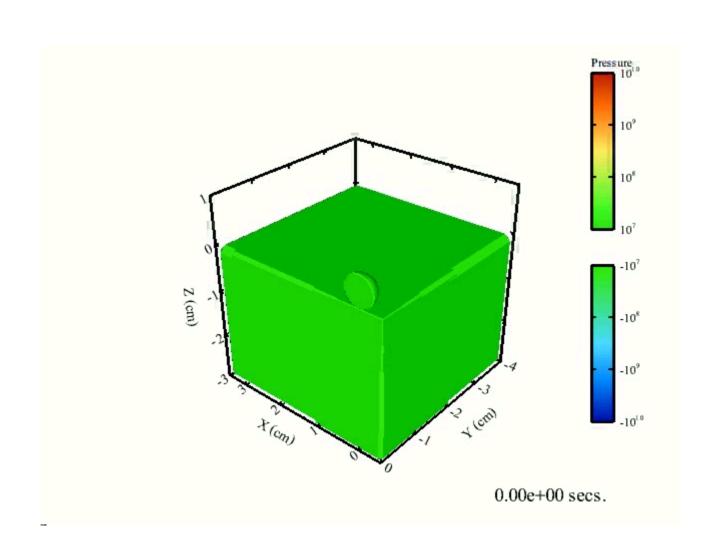
Single Point Initiation: THE MOVIE



Oblique Impact: THE MOVIE



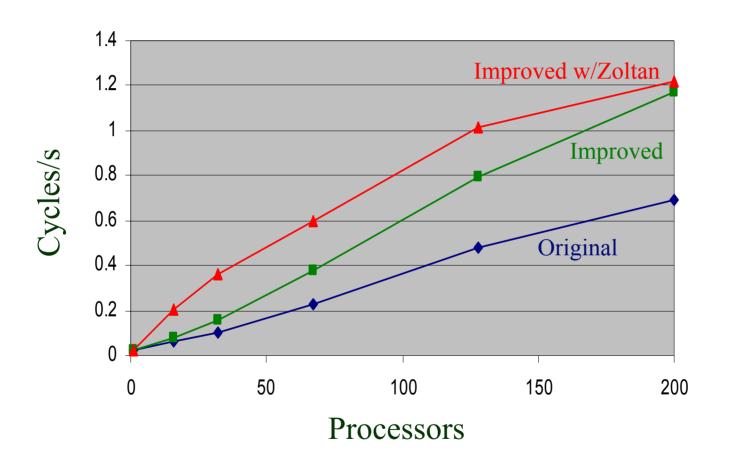
Oblique Impact (cont.): THE MOVIE



Performance Improvements

- Parallel process block refinement/unrefinement as much as possible
 - perform refinement only once every 3 cycles
 - perform unrefinement only once every 6 cycles
 - increase refinement border to 2 cells to accommodate this
- Perform load balancing only when disparity is more than 10%.
- Use Zoltan to minimize off-processor communications.

Performance Improvements



Proposed Code Developments

- Consolidate AMR message passing to reduce latency
- Reduce size of message buffers
 - allocate space for receive buffers only, re-use send buffers
 - update only a few variables at a time
- Allow blocks to allocate space for only those materials needed (CTH U Alegra)
 - presently space is allocated for all materials in every block

Future Code Developments: CTH **U** ALEGRA (w/ Mark Christon)

- Add new structured-region class to ALEGRA.
 - Multiple regions contain blocks of finite-difference cells (equivalent to AMR CTH blocks).
 - Use CTH legacy Fortran to solve physics, constitutive models, etc. within each block.
 - Use C/C++ to handle interface between blocks.
 - Use ALEGRA superstructure to handle memory management, scratch variable allocation, load balancing of elements, etc.
- ALEGRA parser for user input.
- DIATOM for material insertion.
- Spymaster for visualization.



FY01 Department 9232 Review

Stewart Silling



May 30, 2001





FY01 Projects

Methods development

Modeling of friction stir welding NFE/WFO - Boeing

Peridynamics
 MOU, CSRF

CTH/EPIC support MOU

CTH shear band model
 WFO – Army

Applications

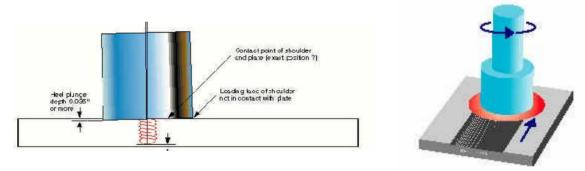
High-G penetrator

Concrete breaching/blasting WFO - Army

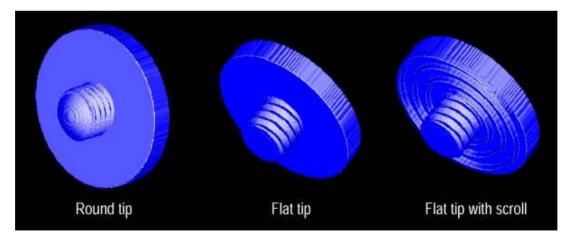
EPW model benchmark DP, MOU

Friction stir welding model

- A new technology that may revolutionize the way planes are built.
- Joins aluminum plates or shells without melting.

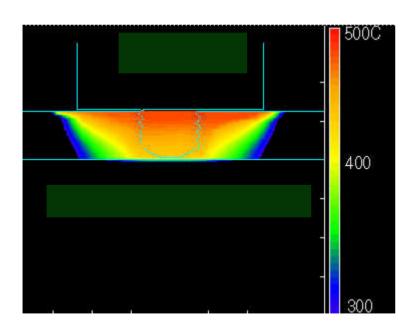


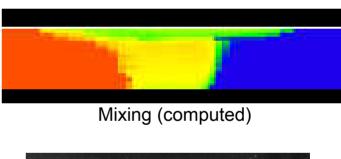
Some tool shapes (CTH model):

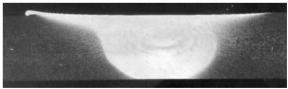


Friction stir welding model: Technical approach

- CTH: prescribe velocities in tool and at mesh boundaries.
- Operator splitting: alternately solve for...
 - Velocities (using CTH)
 - Temperatures (using convection-diffusion solver).



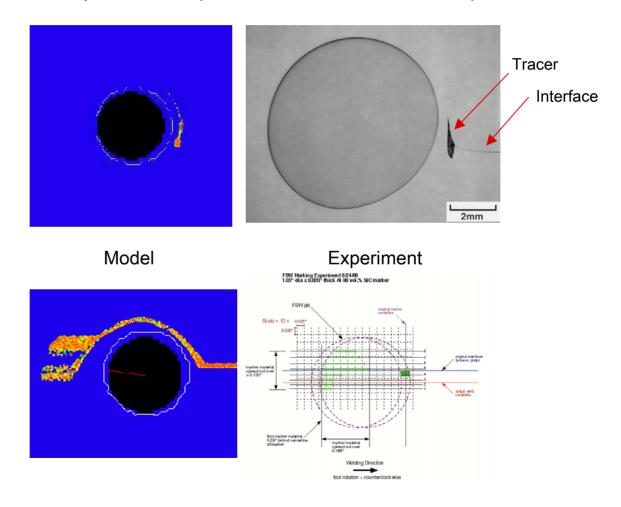




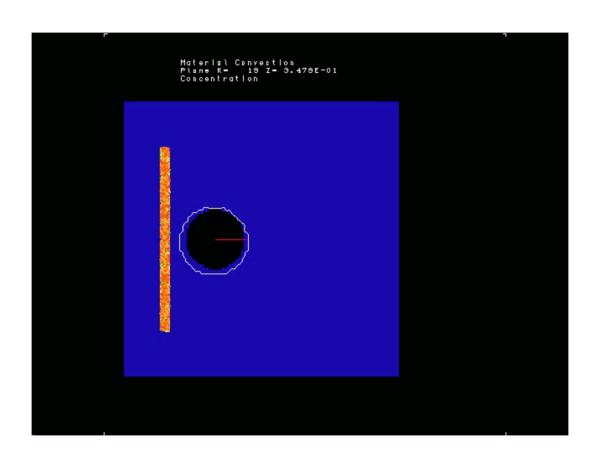
Photograph of cross-section

Friction stir welding model: Typical validation results

• Tracer particle experiments (Rockwell Science Center):



Friction stir welding: THE MOVIE



Friction stir welding model: Status

- A version of the model has been delivered to the sponsor.
 - 16-node SGI
 - 16-node DEC alpha cluster
- This project is critical in establishing a new CRADA with Boeing.
 - This will bring in business to diverse areas at Sandia.
 - Will result in closer relationship between SNL and the aerospace industry.

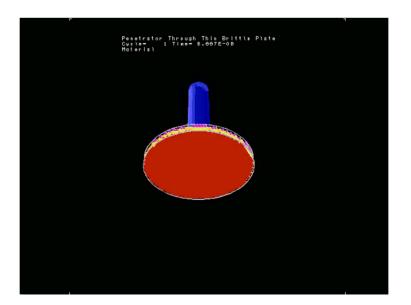
Peridynamic modeling

Objectives

- Develop a theory of continuum mechanics in which the same equations hold on or off of any discontinuities.
- •Provide a useful code based on this theory.

Why

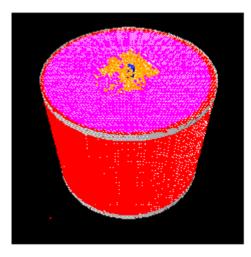
- Enable modeling of spontaneous discontinuities such as cracks without special techniques.
- These singularities are crucial to material failure.



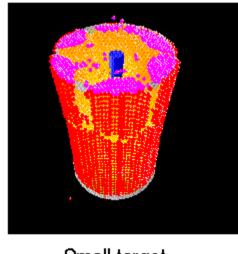
THE MOVIE

Peridynamic applications: Target size effect for earth penetrators

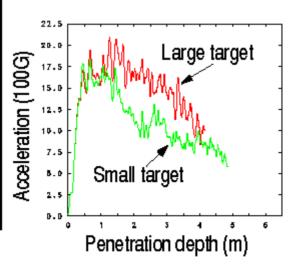
- How big does a target have to be to reproduce half-space response?
- Discrete nature of crack growth has an important effect:



Large target 15 penetrator diameters

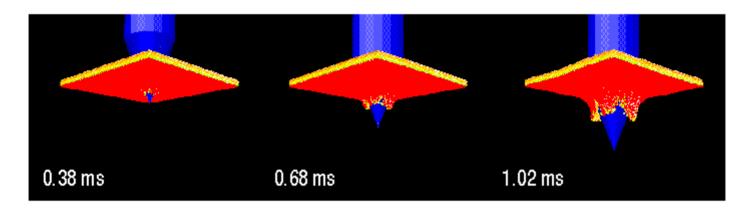


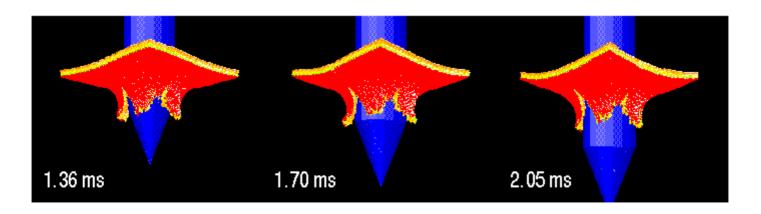
Small target 7.5 penetrator diameters



Peridynamic applications: Petaling

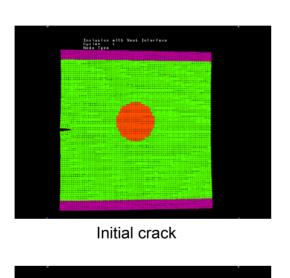
 Perforation of thin ductile plates often results in a family of radial cracks.





Peridynamic applications: Composite material failure

 How do the relative strength of the matrix, fibers, and interfaces affect crack growth?



We did a way but the control of the

Weak fiber

Section in a Yeak Matrix State of the Section of th

Weak matrix



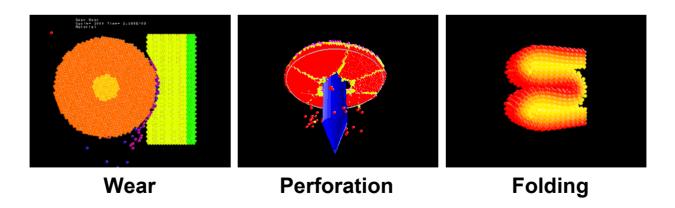
Weak interface

Composite material failure: THE MOVIE



Peridynamic model: Status

- Continuing to develop the theory and code.
 - SNL: fracture mechanics, numerics, code development.
 - MIT: modeling of material defects.
 - Caltech: incorporation of atomistic physics.
- Code is being applied to real-world problems.
 - Potential customers include...
 - ARL: armor
 - Boeing: fatigue cracking, shell impact problems, composites
 - EPW programs: brittle target penetration
 - MEMS: wear, stiction





FY01 Department 9232 Review

Marlin Kipp



May 30, 2001





FY01 Projects

- NEST / Source Term Mitigation ~ Applications to silver surrogates, modern weapon Contributions to field events
- Porous Material Modeling ~ Glass microballoon Explicit pore inclusion / shock response
- Penetration Modeling ~
 WES penetrator / concrete experiments (MOU)
 Other Support ~
 - End point data transfer to monitor component performance in high-fidelity JTA's Shaped charge / structural loads (WFO, w/ 9120)
 - Consistent fragmentation model parameters that represent both sphere impact and shell expansion breakup (NSWC)

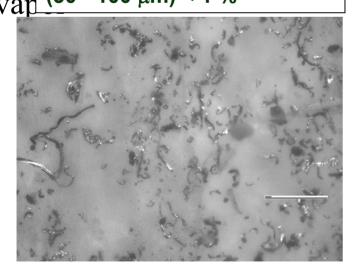
NEST Background

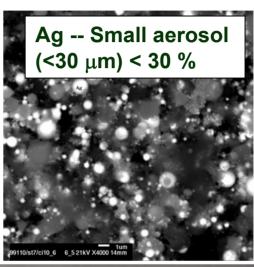
- Use device-specific information on materials and geometry with field tools and/or simulations to assess potential mass fraction of radiological material released as aerosol ($<30\mu m$ aerodynamic)
- Source term aerosol formation from detonated device
 - Prompt formation of solid/liquid/vapor fractions, fragments (Time scale: microseconds)
 - Debris transits explosive products into atmosphere (Time scale: milliseconds)
 - Dispersal of aerosol(Time scale: seconds)
- CTH simulations of devices being used to construct reliable tools for field applications (on-going)

Example of Data Collected in Silver Experiments

• Majority of mass for single shell experiments is large chunks (solid fracture), or small aerosol (liquid breakup, vapor condensation)

• CTH \sim 26% liquid / 1% vapor Da Ag -- Intermediate particles vapor (30 - 100 μ m) < 1%



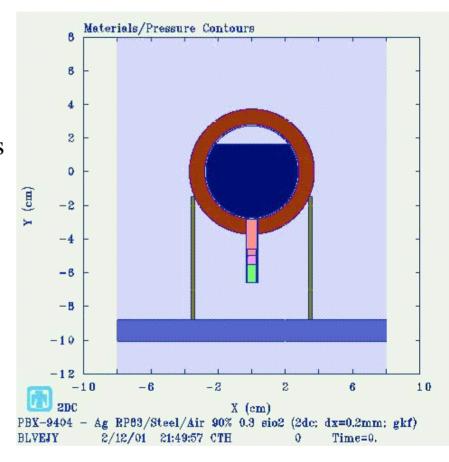




Silver / GMB / PBX-9404 - 2dc CTH

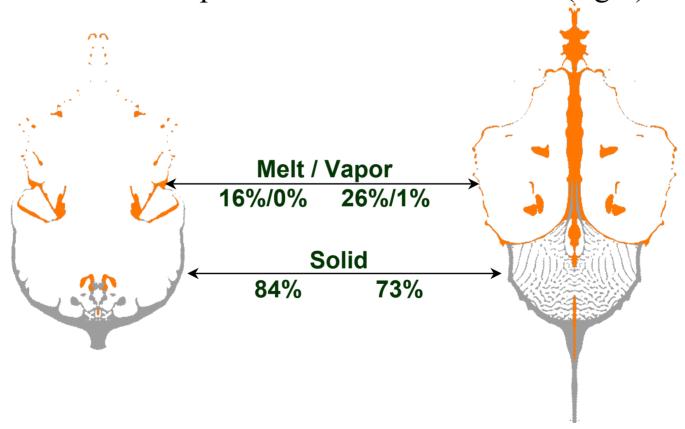
THE MOVIE

- Spherical silver shell (0.9mm, 80g) inside 9mm layer of PBX-9404 (220g)
 - 90% volume fill GMB (24.9g) (porous glass model, 0.3g/cm³)
 - 1-point initiation
- CTH 2dc, $\Delta x=0.2$ mm
 - Presence of glass prevents full collapse of silver
 - Reduces, but does not eliminate,
 fractions of liquid / vapor formed

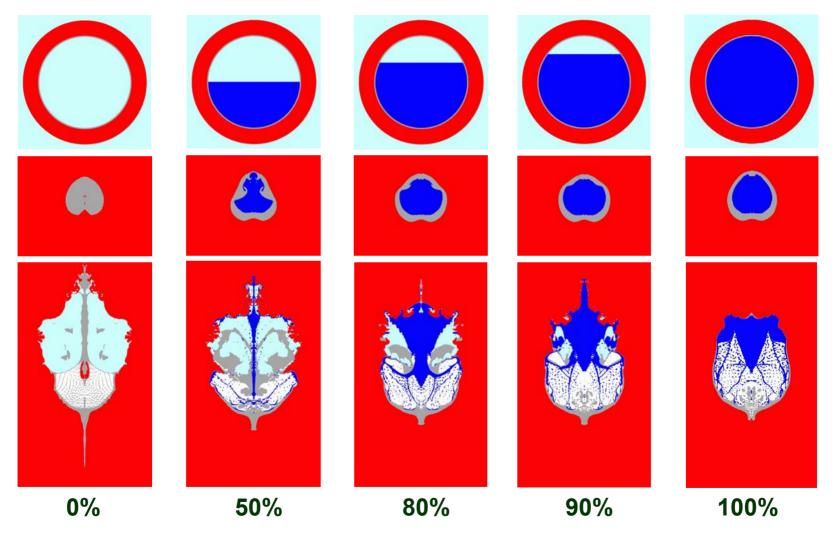


Silver / GMB / PBX-9404 - 2dc CTH

• Presence of 90% GMB fill (left) alters silver expansion characteristics compared with unfilled baseline (right)



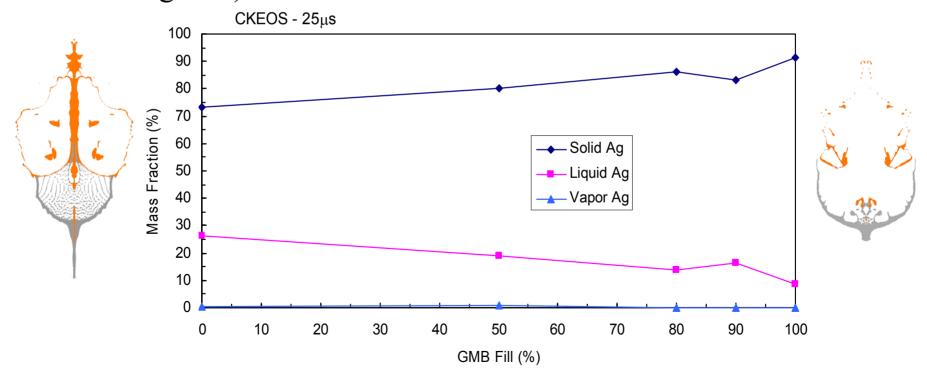
Effects of GMB Fill Volume: 1-Pt Initiation



GMB Fill

Silver Solid/Liquid/Vapor Fractions vs. %GMB

- Increased GMB fill volume generally leads to formation of less liquid / vapor compared to unfilled baseline
- Quartz fill initial density: 0.325g/cm³ (solid density: 2.204g/cm³)



Silver Solid / Liquid Initial Fragment Sizes

Solid - Toughness:
$$S = \left(\frac{\sqrt{24}K}{\rho c \dot{\varepsilon}^2}\right)^{1/3}$$
 Yield: $S = \left(\frac{1.2Y}{\rho \dot{\varepsilon}^2}\right)^{1/2}$

$$S = \left(\frac{48\gamma}{\rho \dot{\varepsilon}^2}\right)^{1/3}$$

Liquid – Toughness:

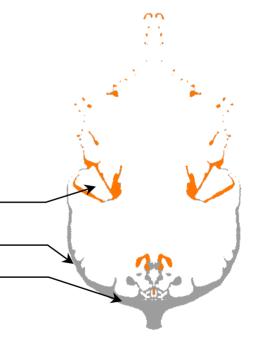
Silver Fragment Sizes / Ejection Velocities

10 - $50\mu m$ (liquid) (2700m/s)

Solid: 1.4mm (shell) - $140\mu m$ (interior) (1000m/s)

Solid: 1.8mm (shell) - 500µm (interior) (800m/s)

(Liquid velocities exceed aerodynamic breakup criteria in explosive product and air environments)



NEST / Source Term Mitigation Summary

- Contributions to field events:
 - Application to LANL hydrotest device ~
 Request to estimate aerosol releases for U / Be materials
 Preliminary results consistent with CTH predictions:
 Some U, no Be aerosol formation
 - SLC Olympics dispersal incident training exercise ~
 Contributed to database of material response to explosive sources (e.g., ceramic fuel rods, toxic metals)
 - Response to concern for potential accident involving a Mk15 lost in the Savannah Delta (Georgia) in the 1950's ~
 Provided estimated source term release of SNM for worst case scenarios.



FY01 Department 9232 Review

Rebecca Brannon

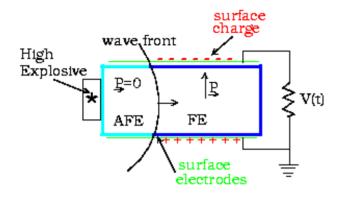


May 30, 2001

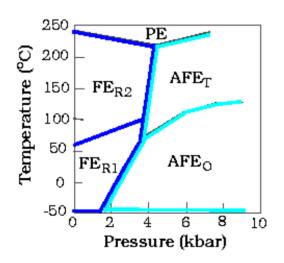




Principle of Power Supply Operation



- Power Supply Operating Principle: Shock-Induced Depoling.
- Phase behavior of PZT is key.
 [phase diagram after Fritz & Keck,
 J.Phys. Chem. 39, 1163 (1978)]

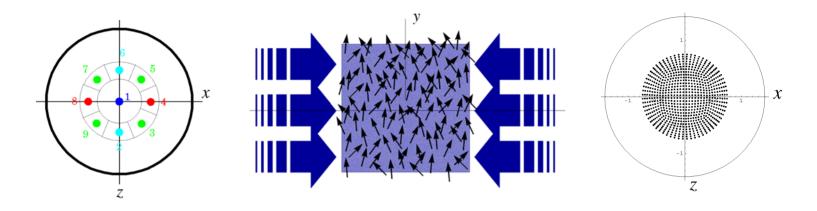


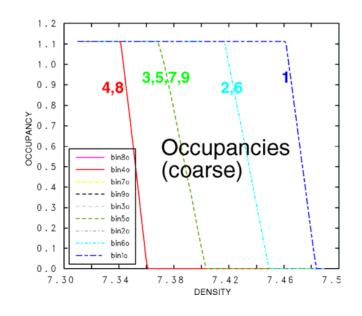
Hallmarks of Ferroelectrics

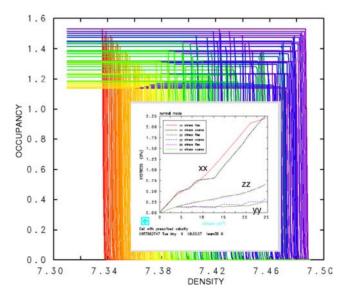
- Spontaneous polarization constrained to specific lattice directions.
- A **DOMAIN** is a region of uniform polarization within a crystal.
- Polarization can switch by twinning under applied stress or E-field



Modeling dipole distributions

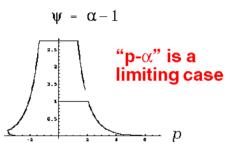


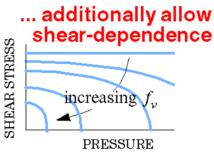


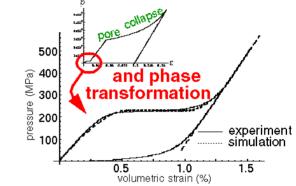




The porosity model







Shear-dependent crush:

$$F(p, \tau, \psi, \varsigma) = 0$$

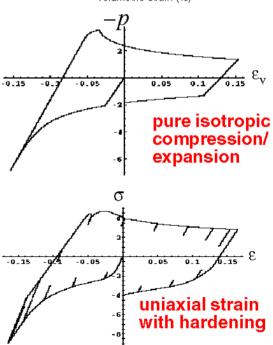
- Positive dissipation $d_p^G = \lambda [F_m \hat{I} + F_s \hat{S}]$.
- Strain-Pore coupling:

$$\dot{\Psi} = (1 + \Psi) \operatorname{tr} d_{\nu}$$

- Nucleation (ad hoc): $\psi^N \propto \frac{\sigma_m}{\epsilon^N K_m (1+w)} 1$
- Consistency: $F_m \dot{\sigma}_m + F_s \dot{\sigma}_s + F_{\psi} \dot{\psi} + F_{\zeta} \dot{\zeta} = 0$.
- Pore-dependent stiffness. $\frac{K}{K} = e^{-\kappa_m \psi}$

Phase transformation:
$$d^T = \dot{r}[T_m\hat{l} + T_s\hat{S}]$$

• Rate dependence: $\dot{\sigma}_{ij}^{\text{over}} = q_{ij} - \frac{\sigma_{ij}^{\text{over}}}{\tau}$

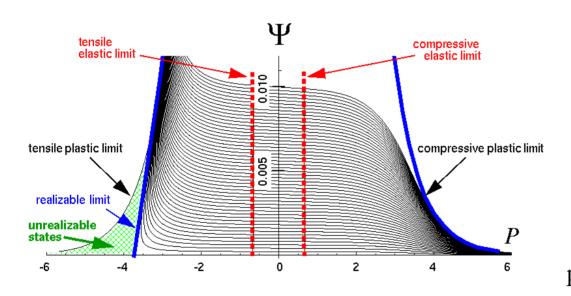


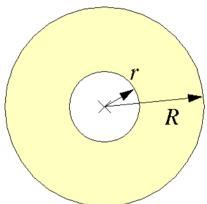




Hollow sphere model: uniform outer pressure P.

Yield begins at the inner radius (elastic limit). Increased pressure propagates the plastic zone to the outer radius (plastic limit).



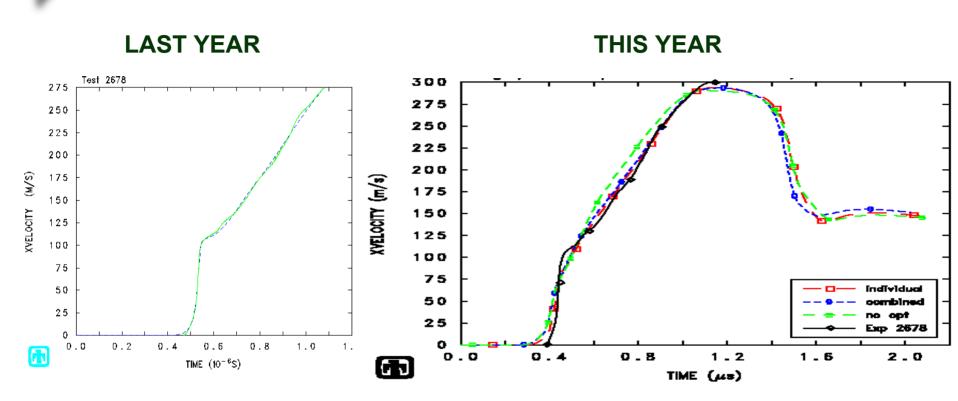


porosity:
$$f = \left(\frac{r}{R}\right)^3$$

pore ratio:
$$\Psi = \frac{f}{1-f}$$

This analytical work proves that the plastic limit curve should not be used to approximate the yield function in tension. Doing so results in an unphysical energy in the macroscale model. However, using the *envelope* is adequate to avoid negative plastic work.

DAKOTA optimization status

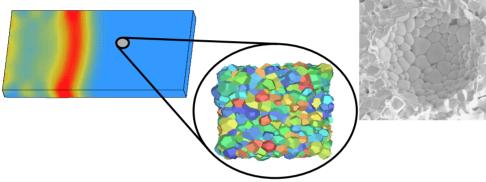


Single-experiment agreement has gone down, but overall test SUITE agreement has improved. DAKOTA optimization has illuminated deficient components in the material model.

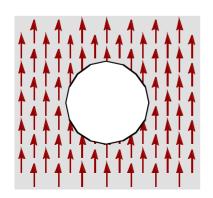


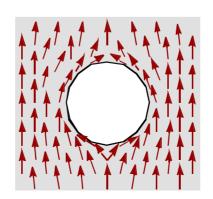
Mesoscale modeling of PZT

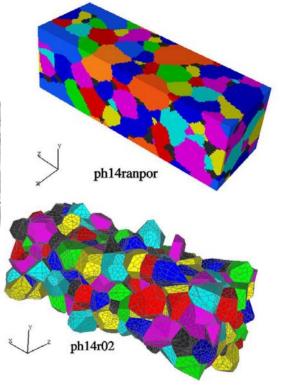
Goal: model shock-induced depoling of PZT at both macro- and meso-scales

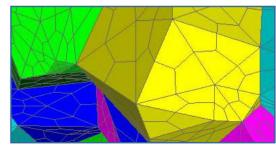


Assign initial occupancies to create a zero divergence field.



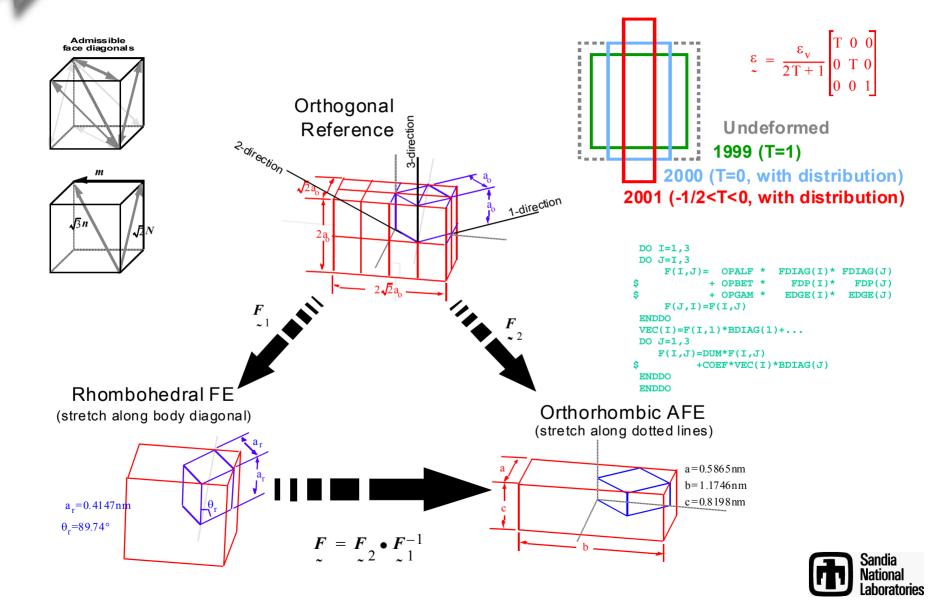








Transformation strain



Mesh-free methods: Motivation

Potential Advantages

- •Better handles large material distortion (no mesh to tangle).
- •Lagrangian particles eliminates constitutive advection errors.
- •Customized shape functions with desired regularity.
- •High rate of convergence.
- Naturally conforming.
- •Easy h- and p- adaptivities.

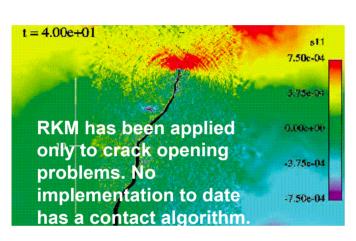
Pervasive Disadvantages

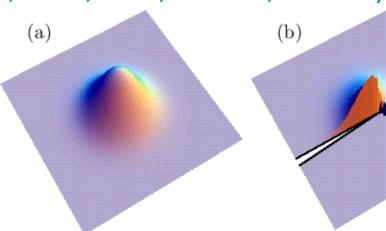
- Complicated boundary treatment.
- •Higher-order shape functions require higher order integration rules.
- •Particle search is usually needed.
- •Boundary detection is required.
- •Large bandwidth in stiffness matrix (RK).
- Continuous field approximation is difficult (often non-interpolating).
- •Galilean and/or Lagrangian invariance is sometimes violated.
- •Finding accurate field gradients is extremely difficult.
- •Handling contact and friction is awkward.



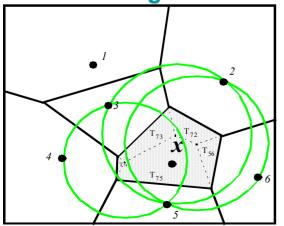
Mesh-Free CONTENDERS

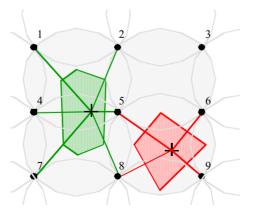
RKM Sandia-Livermore (Klein, Foulk, Chen, Wimmer, and Gao)

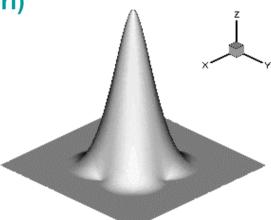




Natural Neighbor Method, LANL (Crane, Shimbri)

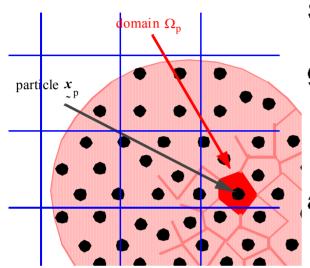








CONTENDER: The Material Point Method (MPM)

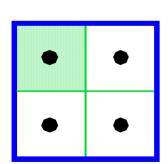


Standard weak formulation applies on the

grid:
$$\sum_{j=1}^{n} m_{ij} \mathbf{a}_{j}(t) = \mathbf{f}_{i}^{int}(t) + \mathbf{f}_{i}^{ext}(t)$$
, where

$$m_{ij} \equiv \int\limits_{\Omega} N_i(\boldsymbol{x}) N_j(\boldsymbol{x}) \rho \, dV \ , \qquad \boldsymbol{f}_i^{\rm int}(t) = - \int\limits_{\Omega} \boldsymbol{g}^s \bullet \boldsymbol{G}_i(\boldsymbol{x}) \rho \, dV \ , \label{eq:mij}$$

$$\mathbf{f}_{i}^{\text{ext}}(t) = \int_{\partial \Omega_{T}} \mathbf{T} N_{i}(\mathfrak{g}) dS + \int_{\Omega} N_{i}(\mathfrak{g}) \mathbf{b} \rho dV .$$



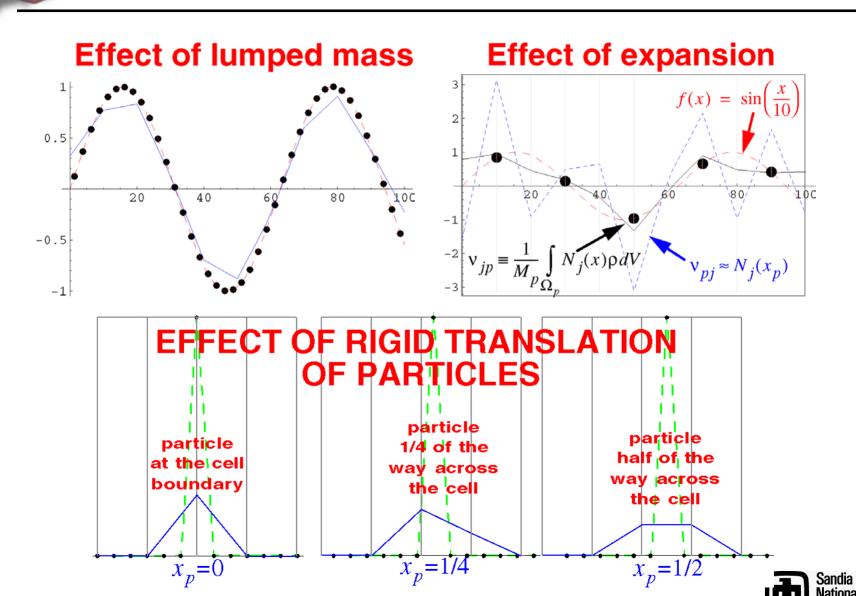
For FEM, Gauss points are used to compute these integrals.

However, for the MPM,

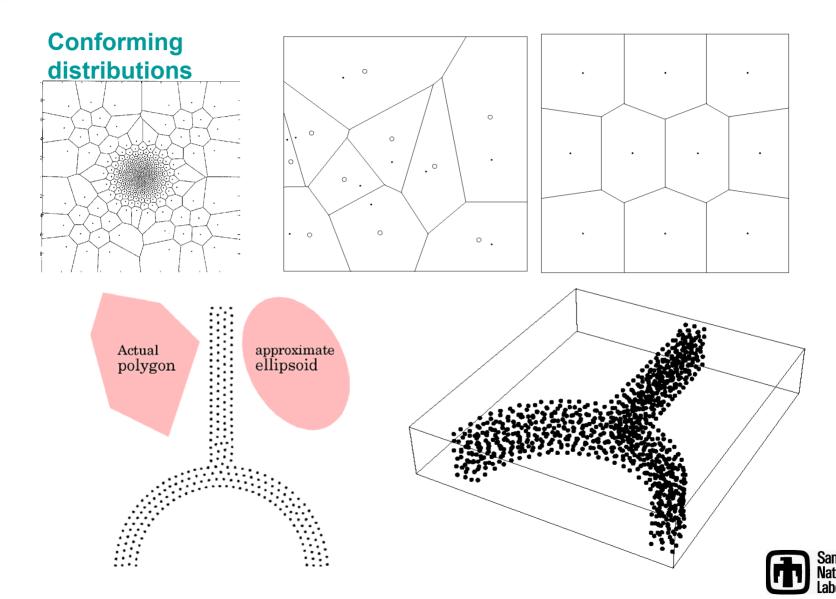
$$\int_{\Omega} f(\mathbf{x}) \rho dV = \sum_{p=1}^{N} \int_{\Omega p} f(\mathbf{x}) \rho dV \approx \sum_{p=1}^{N} f_{p} M_{p}$$



MPM (implied) particle basis



Centroidal Voronoi distributions





In summary, ...



we are

 15 professionals with ~270 years of combined experience,





who work

 in the area of shock physics and M&S environments,





ranging from

 research to development to application to support, and





funded by

 a large and diverse customer base.







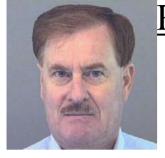












Ray Bell

- BS Physics University of Arizona
 Graduate work University of Florida thru Eglin AFB
- Major USAF, ret. (7 years hydrocode dev. and app.)
 11 years@ NMERI/S3 (hydrocode dev. & app.),
 4 years@ SNL (hydrocode dev. & app.)
- 3 kids ranging in age from 13 to 31, and 2 grandkids



Rebecca Brannon

- BS ME UNM
 MS/PhD Engineering Mechanics U of Wis., Madison
- 8 years @ SNL (Comp. Physics)
- Likes juggling, watching movies, square dancing, skiing, teaching motorcycle safety, collecting puzzles, and reciting "geeky" poetry, Nintendo fanatic



Pat Chavez

- BS Math & Physics NM Tech, MS Applied Math - RPI, PhD Applied Math - Cornell
- 25 years @ SNL (Comp. Physics, CAD/CAM/CAE, TDY/NIST, NWSBU, Comp. Physics)
- Master Gamer ('98 USA finals, '98 World finals hold/officiate tourneys) & Paintballer



Bob Cole

- BS ME Tulane, MS Engineering Mechanics - VPI ABD Numerical Methods - Tulane
- 7 years @ US Navy Surface Weapons Center (gun M&S), 13 years @ Waterways Experimental Station (hydro code), 7 years @ Private Sector (hydro code dev./app.), 3 years @ NMERI (WIPP),
 - 3 years @ SNL (Comp. Physics)
- Met wife at Mardi Gras 33 years ago; still counting after 3 grown children & 2 grandchildren. Cannot run for President, even if I wanted to; the US constitution so states.



Dave Crawford

- ScB/PhD Physics Brown
- 8 years @ SNL (Comp. Physics)
- I remember as a kid thinking that I may one day go to the Moon and that by 2000 we would certainly have landed on Mars. Do we really want to be remembered as the generation that saved social security yet our greatest space-based achievement is to build a condominium a mere 200 miles away?



Paul Demmie

- BS, PhD Physics Univ. of Pittsburgh, Sandia Certificate of Computer Simulation
- 5 years @ Univ. of Pitts. (Professor of Math & Physics),
 7 Years @ EG&G Idaho (Nuclear Reactor Safety),
 17 Years @ SNL (NR Safety, BMD, NW Surety, Comp. Phys)
- Plays cello/chamber orchestra and enjoys photography



Millie Elrick

- BS Engineering Physics Montana State MS Physics - Lehigh
- Last 12 years working on CTH
- My first Social Security check arrives in March



Archie Farnsworth

- BS/MS Engineering Science/Mechanics ASU, PhD Engineering Brown
- 31 years @ SNL (NW Enviro. Testing, Inertial Fusion Target Design, Nuclear Weapon Effects, Optical Initiation of HE, Optical Signatures)
- Father of 7, grandfather of 9, CLDS Leader (Bishop)



Marlin Kipp

- BS Engineering Mechanics Lehigh MS/PhD Applied Mechanics - Lehigh
- 27 years @ SNL (Comp. Physics dynamic fracture and fragmentation, reactive models for explosives, NG standoff simulations, explicit simulations with foam, debris clouds, granular explosives, and concrete)
- Bicycle commuter (>50K miles), hiker (likes Colorado 14'er walkups), woodworker (chairs, tables, beds, etc.)



Jason Libersky

- BS Biology NM Tech,
 BS Astrophysics UNM,
 BS Religion UNM
- 5 years as Surgical Assistant/Organ Procurement,
 2 years as Environmental Engineer,
 2 years at SNL (student intern Comp. Physics)
- Plays cello, loves to cook and write

Marilyn Murray

- 1/2 BA degree in Business
- 20+ years of secretarial experience (UC-Boulder, UW-Madison, NMSU, Rice, UNM in the areas of Criminal Justice, Agronomy, Philosophy, Engineering, NASA Relations, Ecology and Evolutionary Biology, etc) 5+ years @ SNL (Security, Comp. Physics)
- Blessed to grow up on a farm where I was a typical 4-H kid including raising my horses (Dolly & Darling) and helping with farm chores (planting, harvesting, transporting)

Stewart Silling

- BS NE/Physics MIT, M Eng. NE - Berkeley, PhD Applied Mechanics - CalTech
- 3 years @ SAIC (beltway bandit),
 2 years @ NRC (nuclear waste regulator),
 3 years @ Brown University (Professor),
 10 years @ SNL (Comp. Physics)
- Father of twins, cat fancier, and railroad nut



Paul Taylor

- BS/MS Engineering Mechanics Penn State PhD Theo. & App. Mechanics, University of Illinois
- 20 years @ SNL (Solid State Science simulation & study of material behavior on atomic length scales, Comp. Physics constitutive model development, hydrocode development, CTH development lead)
- "Jack" of many pleasures/trades boating (sail & power), skiing (water & snow), scuba diving, flying, vintage car restoration, home improvement